LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.456	247	251	264	rVB	716833	1390720	59.96%	6.953%
2	4.947	291	294	296	rBV	1837287	2255996	97.27%	11.280%
3	6.056	388	391	393	rBV	1989515	2290588	98.76%	11.453%
4	6.159	397	400	402	rBV	1867942	2231338	96.21%	11.156%
5	6.387	418	420	422	rBV	443767	377052	16.26%	1.885%
6	6.547	431	434	436	rBV	1404004	1645183	70.94%	8.226%
7	6.970	468	471	473	rBV	970972	1471081	63.43%	7.355%
8	7.679	530	533	535	rBV	491303	492429	21.23%	2.462%
9	8.765	624	628	630	rBV	1856400	2319275	100.00%	11.596%
10	9.165	660	663	665	rVB	303637	295129	12.73%	1.476%
11	9.416	682	685	687	rVB	586447	515586	22.23%	2.578%
12	10.193	751	753	756	rBV2	920011	1236809	53.33%	6.184%
13	10.353	765	767	772	rBV	20922	27092	1.17%	0.135%
14	10.879	811	813	815	rBV	640208	526817	22.71%	2.634%
15	11.154	835	837	841	rBV	33086	60350	2.60%	0.302%
16	11.222	841	843	845	rVB	20148	25928	1.12%	0.130%
17	11.451	861	863	867	rBV2	61956	86943	3.75%	0.435%
18	11.531	869	870	873	rVB	21230	26730	1.15%	0.134%
19	12.468	949	952	954	rBV	1763504	1678674	72.38%	8.393%
20	13.394	1030	1033	1039	rBV	123815	247108	10.65%	1.236%
21	13.485	1039	1041	1044	rVV	450755	415167	17.90%	2.076%
22	14.800	1153	1156	1158	rBV	313073	326256	14.07%	1.631%
23	15.257	1193	1196	1207	rBV3	16481	58205	2.51%	0.291%

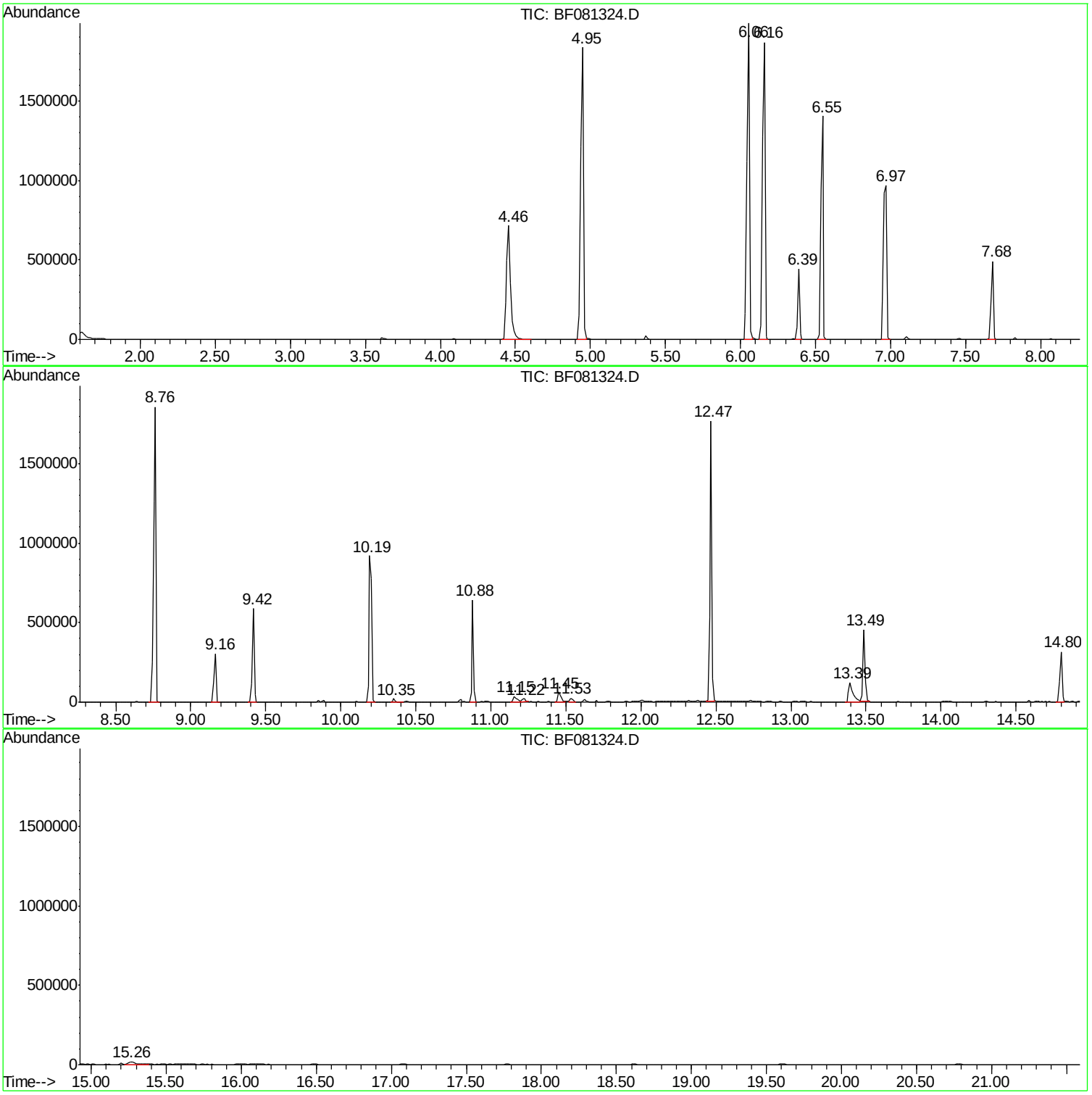
Sum of corrected areas: 20000456

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

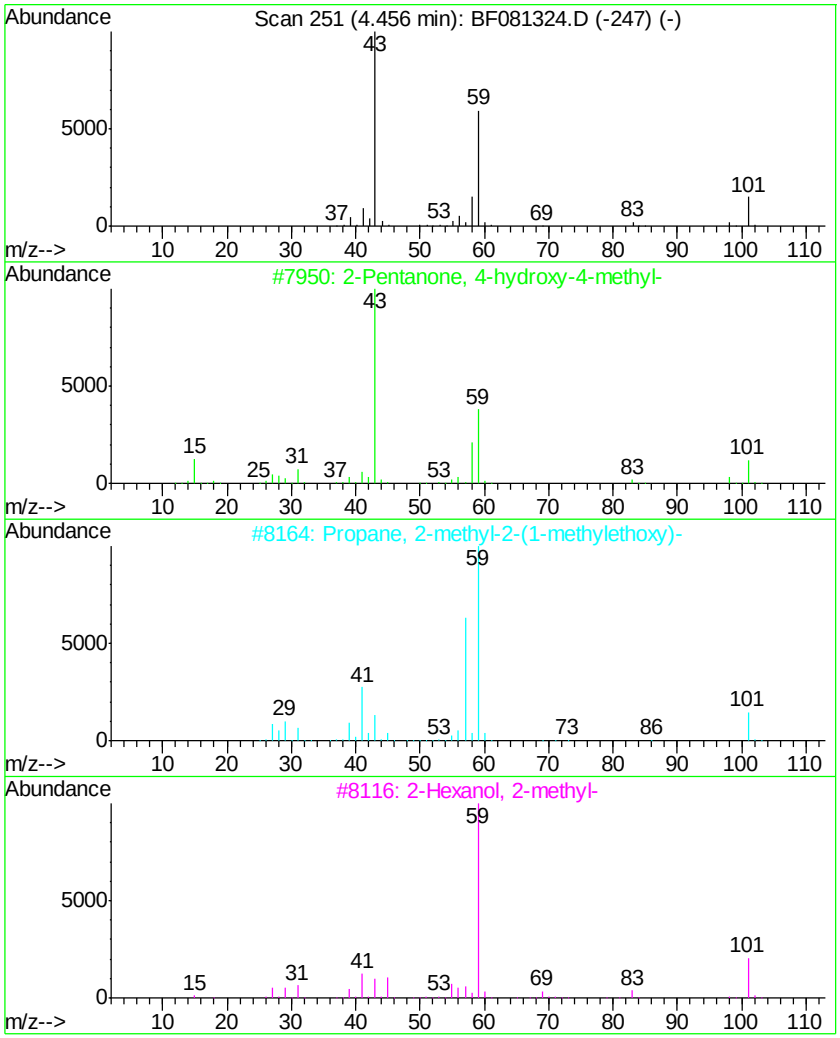
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

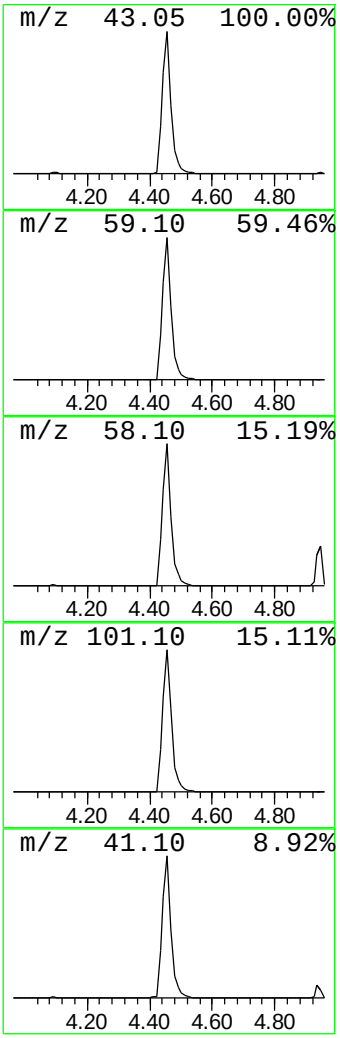
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	73.77 ng	1390720	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

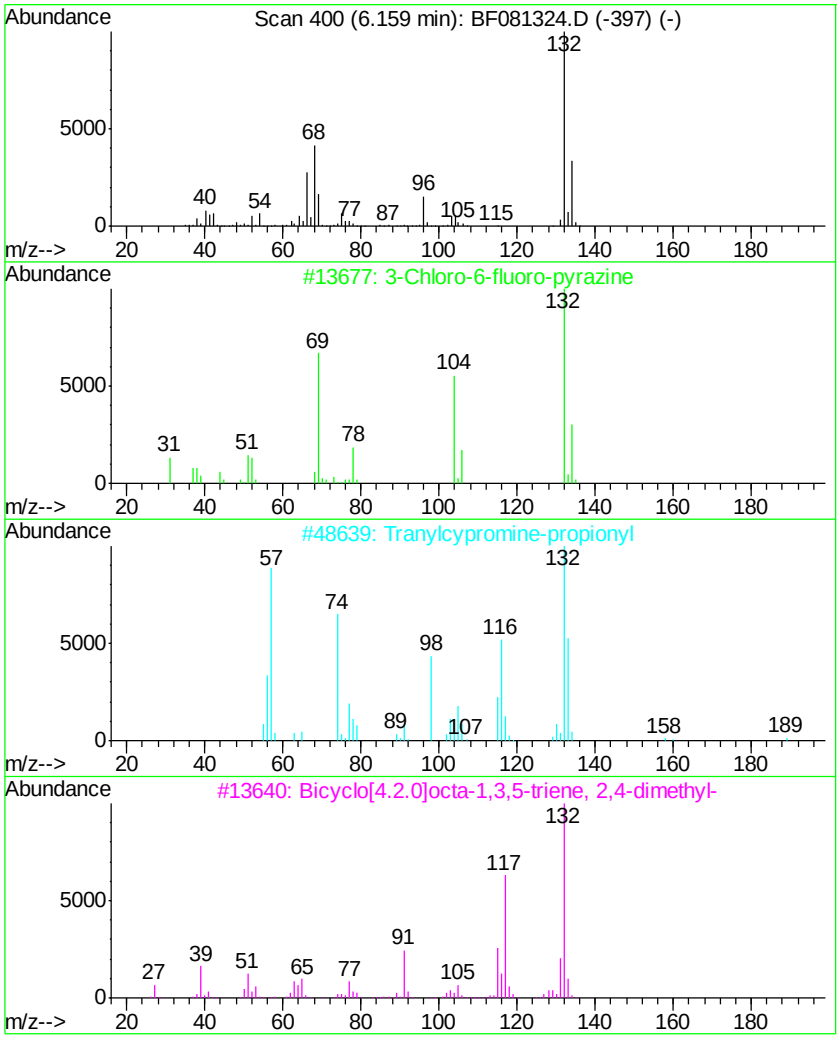
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

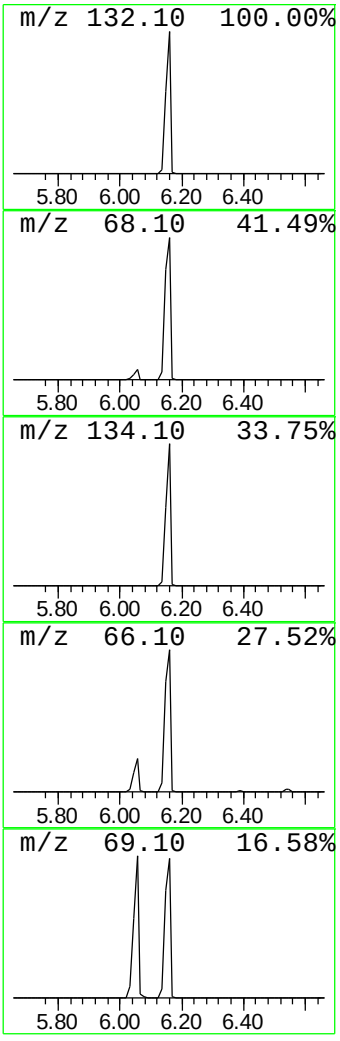
****

Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	118.36 ng	2231340	1,4-Dichlorobenzene-d4	6.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

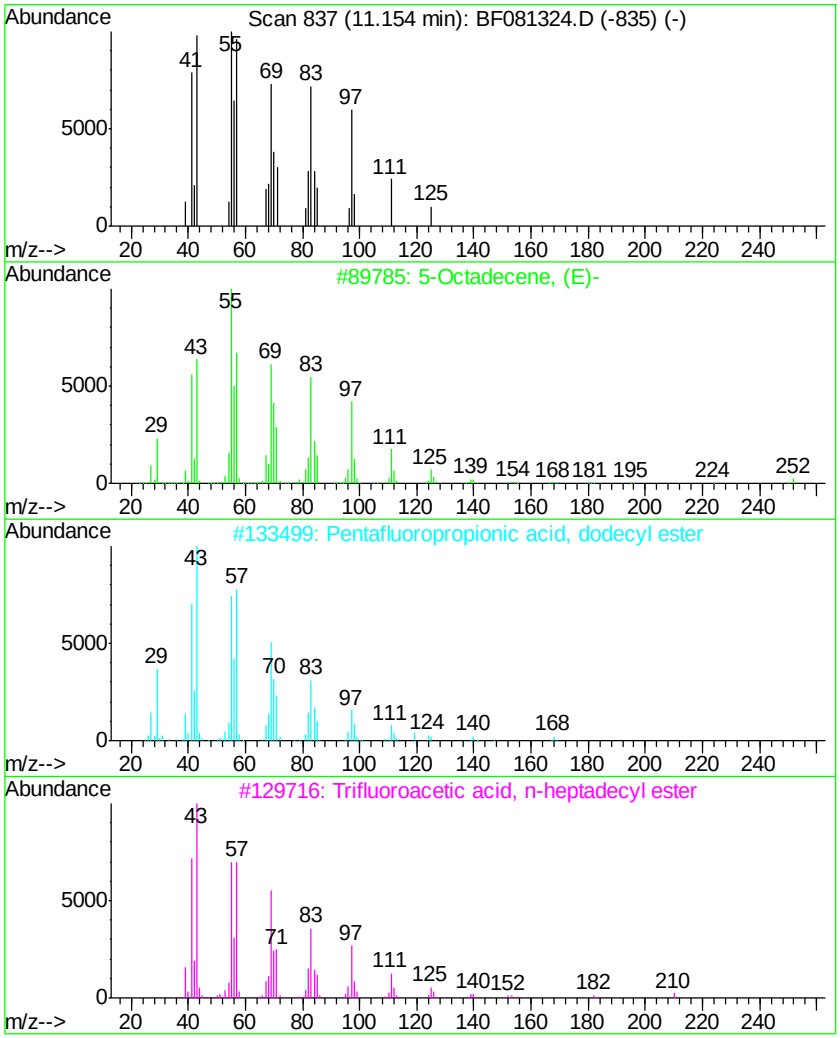
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

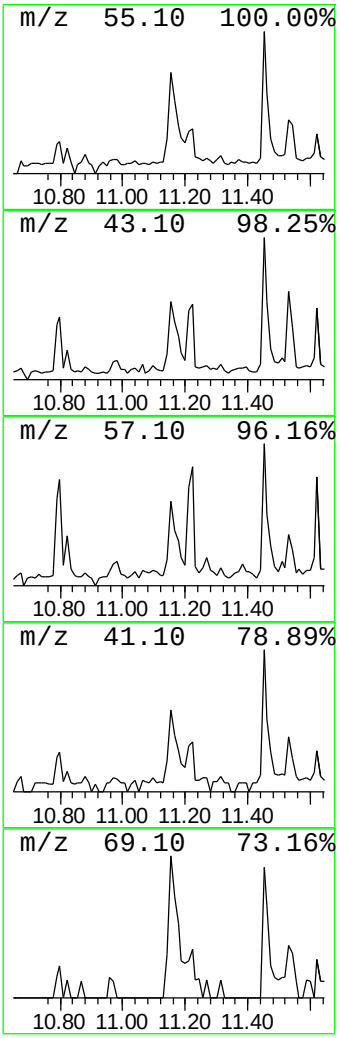
****

Peak Number 4 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	2.29 ng	60350	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
2	Pentafluoropropionic acid, dodec...	332	C15H25F5O2	006222-04-4	87
3	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	86
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	78
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	78





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

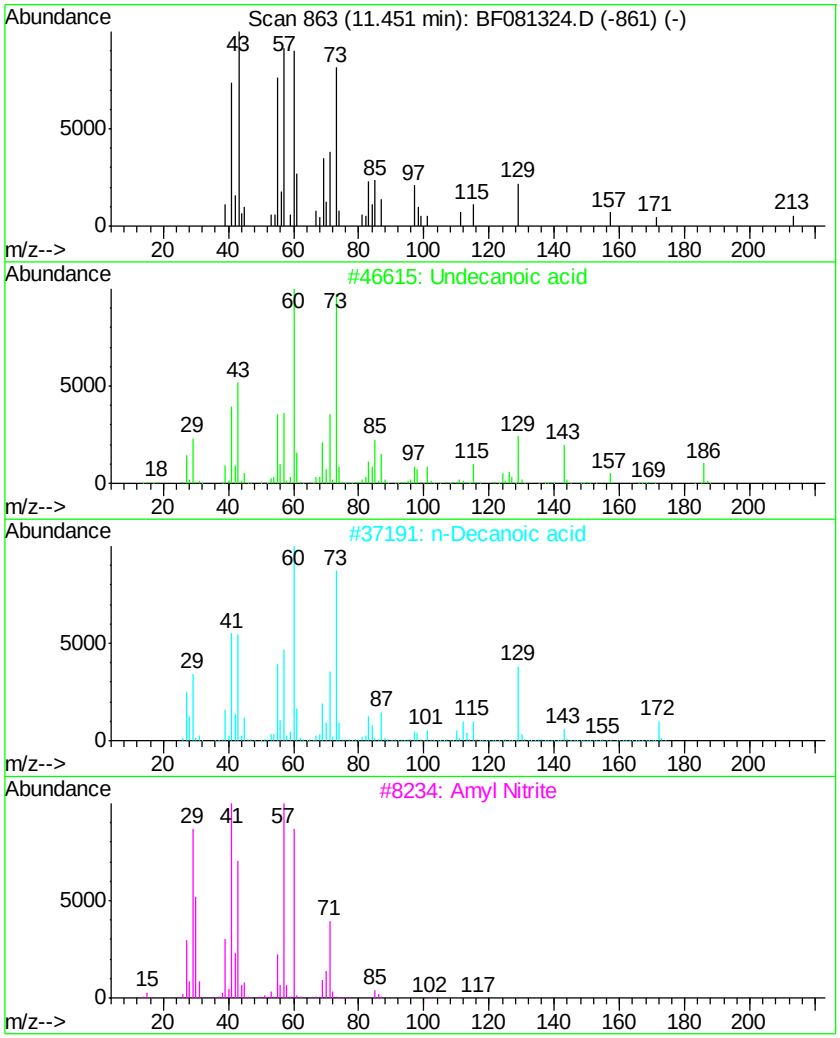
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

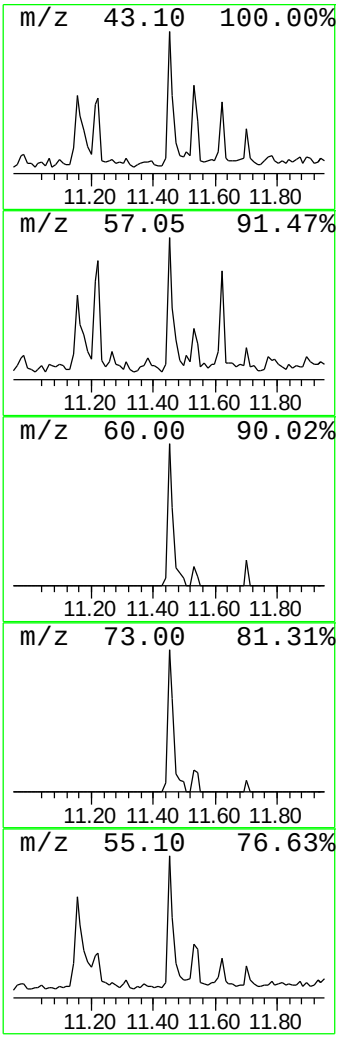
****

Peak Number 5 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	3.30 ng	86943	Phenanthrene-d10	10.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	78
2	n-Decanoic acid	172	C10H20O2	000334-48-5	59
3	Amyl Nitrite	117	C5H11NO2	000110-46-3	38
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	22
5	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	22





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

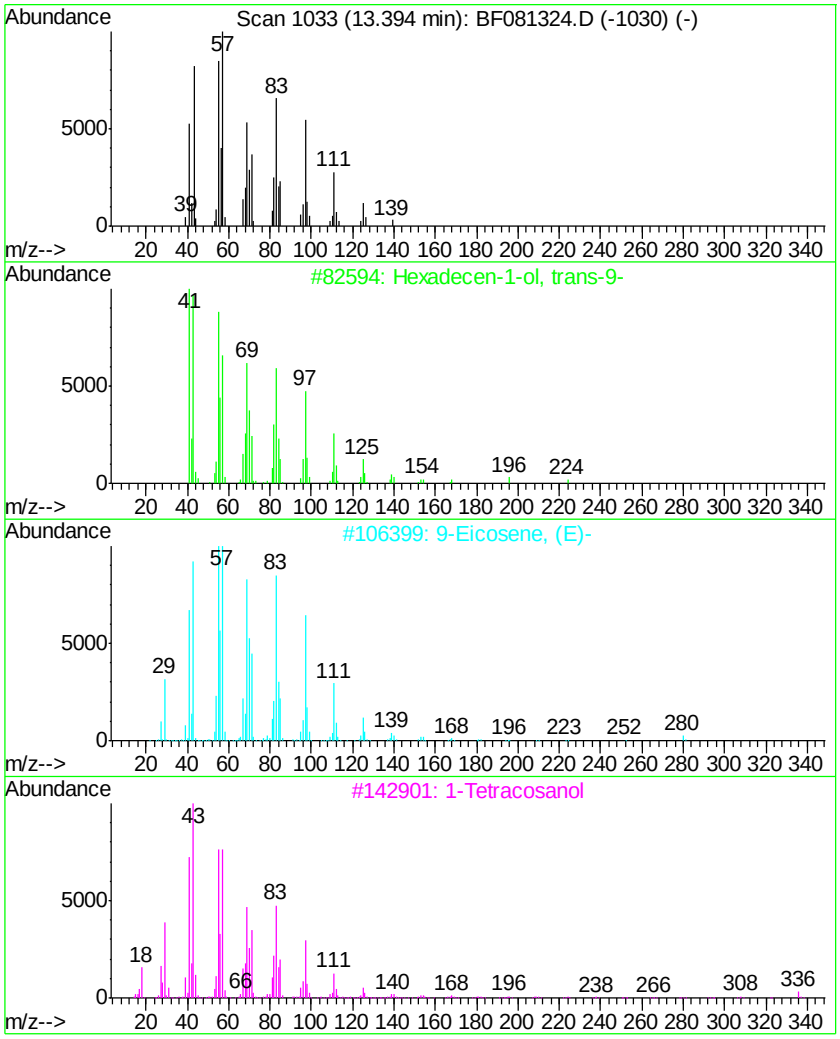
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

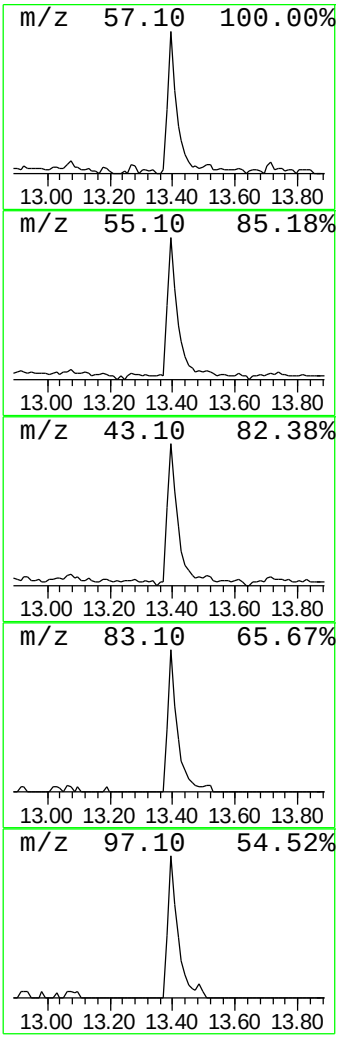
****

Peak Number 6 Hexadecen-1-ol, trans-9- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.39	11.90 ng	247108	Chrysene-d12	13.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	90
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	87
3	1-Tetracosanol	354	C24H50O	000506-51-4	87
4	5-Eicosene, (E)-	280	C20H40	074685-30-6	81
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

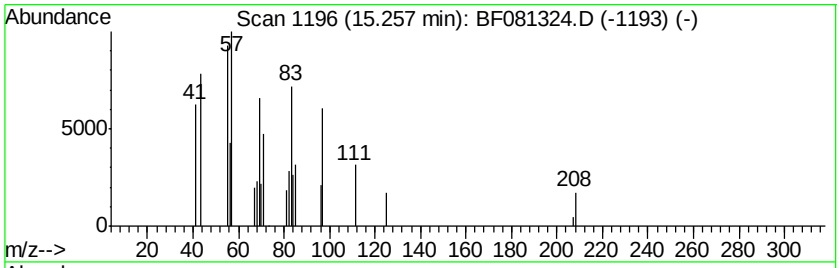
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

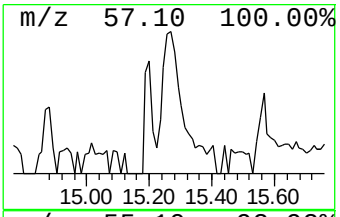
****

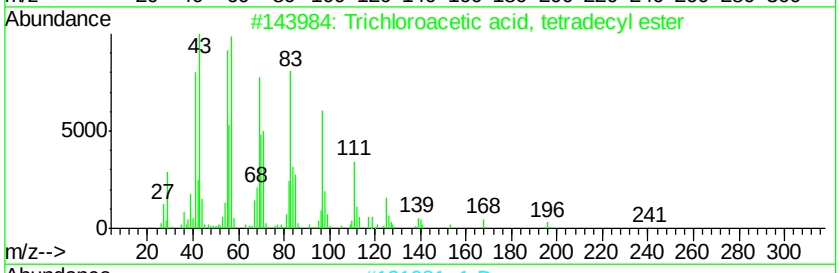
Peak Number 7 Trichloroacetic acid, tetra... Concentration Rank 5

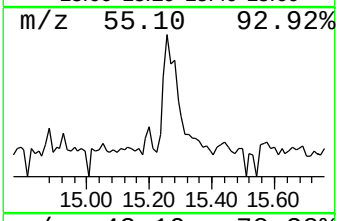
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	3.57 ng	58205	Perylene-d12	14.80

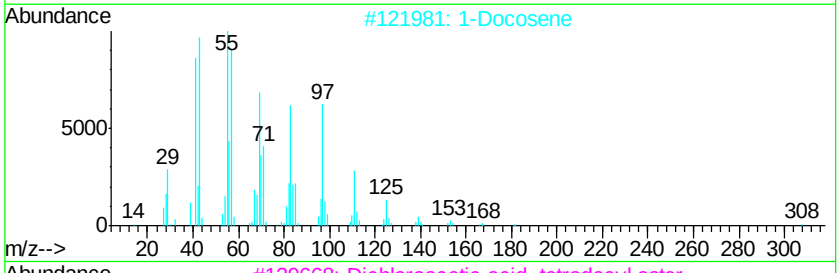
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
2	1-Docosene	308	C22H44	001599-67-3	86
3	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	86
4	17-Pentatriacontene	491	C35H70	006971-40-0	83
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83

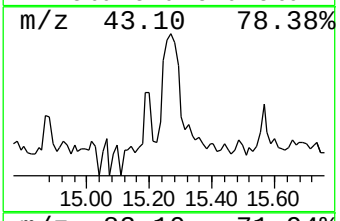


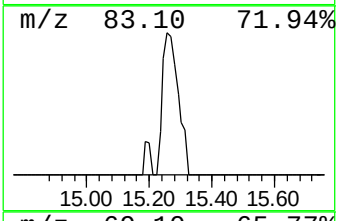


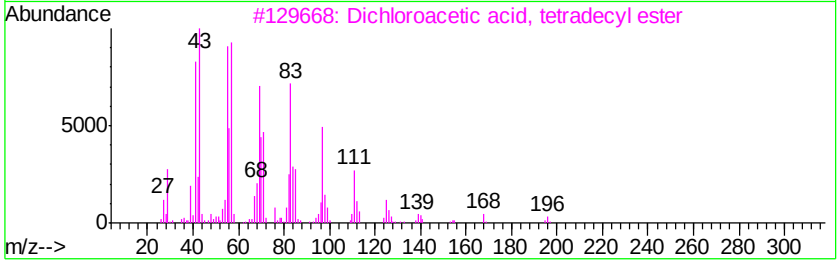


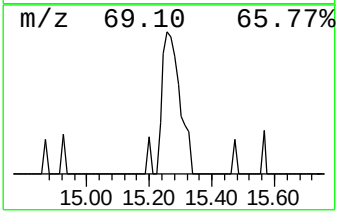












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
Data File : BF081324.D
Acq On : 2 Sep 2015 1:46
Operator : UM/IZ
Sample : G3479-13
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COFF-3-7(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.46	73.8	ng	1390720	1	6.39	377052	20.0
unknown6.16	6.16	118.4	ng	2231340	1	6.39	377052	20.0
5-Octadecene, (E)-	11.15	2.3	ng	60350	4	10.88	526817	20.0
Undecanoic acid	11.45	3.3	ng	86943	4	10.88	526817	20.0
Hexadecen-1-ol, t...	13.39	11.9	ng	247108	5	13.49	415167	20.0
Trichloroacetic a...	15.26	3.6	ng	58205	6	14.80	326256	20.0